

Corrigendum:

Corrigendum to [Synthesis of core-shell nanoparticles Si-ZnS by reactive deposition of photocatalytic ZnS layer on the surface of carrier Si nanoparticles in aerosol microdrops].

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2.2. Theoretical background of concrete application for core-shell particles Si-ZnS

Zinc sulfide which will form the shell of the particles will be prepared by precipitation reaction in aqueous solutions of 1 mmol.L⁻¹ zinc acetate and 6 mmol.L⁻¹ sodium sulphide.



Our aim is to limit the scope of local reactions by microvolume of aerosol drop. This aerosol drop is formed by dispersion of Si nanoparticles in zinc acetate solution. The aim is the preparation of aerosol drop with a concentration of Zn(Ac)₂ which will lead to the formation of the ZnS shell with desired thickness h . Concentration c_{solids} weight of Si nanoparticles will be obtained by weighing the dry matter m_{solids} by evaporation analysis. At known density $\rho_{\text{solids}} = \rho_{\text{Si}}$ then we can express the volume fraction of dry matter in the liquid silicon nanoparticles by equation (2)

$$c_{\text{solids}} = \frac{m_{\text{solids}}}{V_{\text{liquid}} + V_{\text{solids}}} \approx \rho_{\text{solids}} \frac{V_{\text{solids}}}{V_{\text{liquid}}} \rightarrow V_{\text{solids}} \approx \frac{c_{\text{solids}}}{\rho_{\text{solids}}} V_{\text{liquid}} \quad (2)$$

If we know the statistical size distribution of nanoparticles $P_v(v_i)$ then the total volume $V(v_i)$ size fraction v_i of Si dry matter is expressed by equation (3)

$$P_v(v_i) = \frac{V(v_i)}{\sum_{j=1}^m V(v_j) = V_{\text{solids}}} \rightarrow V(v_i) = V_{\text{solids}} P_v(v_i). \quad (3)$$

At spherical approximation of the shape of nanoparticles the ratio between volume and surface is uniquely determined and the volume fraction of the total surface v_i in the volume of liquid V_{liquid} applies:

$$S(v_i) = 6 \frac{c_{\text{solids}}}{\rho_{\text{solids}}} V_{\text{liquid}} \frac{P_v(v_i)}{d_i}. \quad (4)$$

The total surface of Si particles for volume of aerosol dispersion of spherical drop is given by relation:

$$V_{\text{liquid}} = \frac{4}{3} \pi R^3 \rightarrow S(R) = \frac{8\pi R^3 c_{\text{solids}}}{\rho_{\text{solids}}} \sum_{i=1}^m \frac{P_v(v_i)}{d_i}. \quad (5)$$

If we require the thickness of the shell h then in a simplified approximation $V_{\text{shell}} = h \cdot S(R)$ the total mass m_{shell} of ZnS shell is given by equation (8)

$$m_{\text{shell}} = \rho_{\text{shell}} V_{\text{shell}} = \rho_{\text{shell}} \cdot h \cdot S(R) = 8\pi R^3 h c_{\text{solids}} \frac{\rho_{\text{shell}}}{\rho_{\text{solids}}} \sum_{i=1}^m \frac{P_v(v_i)}{d_i} \quad (6)$$

Coefficient of proportionality κ between the molar masses also determines the relation between the general masses of reactants $M_{\text{Zn(Ac)}_2} = \kappa \cdot M_{\text{ZnS}} \leftrightarrow m_{\text{Zn(Ac)}_2} = \kappa \cdot m_{\text{ZnS}}$. By its use we can calculate the concentration of Zn(Ac)_2 necessary for the formation of ZnS shell with thickness h :

$$c_{\text{Zn(Ac)}_2} = \frac{m_{\text{Zn(Ac)}_2}}{V_{\text{liquid}}} = 6\kappa h c_{\text{solids}} \frac{\rho_{\text{ZnS}}}{\rho_{\text{solids}}} \sum_{i=1}^m \frac{P_v(v_i)}{d_i}. \quad (7)$$

At size distribution of Si carrier particles as mentioned in the experimental section below and the thickness of the desired shell ZnS $h = 20$ nm and $\kappa = 1.88$ we obtained concentration $c_{\text{Zn(Ac)}_2} \approx 5$ g/l.